Available online at www.sciencedirect.com
ScienceDirect
Journal of Power Sources 162 (2006) 992–1002
JOURNAL OF POWER SOURCES
www.elsevier.com/locate/jpowsour

Three-dimensional, two-phase, CFD model for the design of a direct methanol fuel cell

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Received 11 April 2006; accepted 26 July 2006
Available online 18 September 2006

Abstract

This study presents a computational fluid dynamics (CFD) model for modelling gas evolution and current distribution in a direct methanol fuel cell (DMFC). The improved two-phase model includes a new sub-model for estimating the interface mass transfer without empirical correlations. Simulation results in a horizontal channel of the DMFC agree with typical trends reported in the literature for bubbly flows. The increase in inlet flow rate is found to lead to a decrease in the gas content in the outlet of the anode channels. A case study illustrates applications of the CFD model for modelling gas evolution and current distribution in a DMFC with a parallel flow-field design. Simulation results with a improved two-phase model provide an explanation of experimental observations of a transparent DMFC with parallel channels. An improved three-dimensional CFD model includes all relevant phenomena and is valuable for gas management in a DMFC design.

Keywords: Direct methanol fuel cell; Two-phase model; Gas management; Flow-field design; Computational fluid dynamics

1. Introduction

Understanding a two-phase phenomenon is important for designing a high-performance direct methanol fuel cell (DMFC). Critical issues for improving the DMFC performance are methanol crossover, gas management on the anode side, and water management on the cathode side. Gas management is especially important in a DMFC design since the methanol electrochemical oxidation produces carbon dioxide flux on the anode side. Removing CO_2 bubbles is required to avoid blocking anode channels that may lead to limited mass transport.

A number of physicochemical phenomena take place in a DMFC, including momentum and mass transfer, electrochemical reactions, and gas–liquid flow in the anode and cathode channels. All these processes are coupled and result in a need for optimum cell design and optimum operating conditions. Thus, good understanding of these complex, interacting phenomena is essential in fuel cell design.

Researches devoted to exploring mass transfer and electrochemical reactions in DMFCs are numerous [1–11]. Scott et al. [1] examined the feasibility of using stainless-steel mesh materials as flow beds. They reported electrochemical performance and gas management characteristics with flow-beds from flow visualization studies on the anode side. Geiger et al. [2] used neutron radiography to investigate of gas-evolution patterns in anode flow-fields. It was found that gas accumulates to a large extent at the inner section of spiral channels and thereby blocks a considerable part of the active area. They noted that a spiral type of flow-field is not appropriate for the anode. Argyropoulos et al. [3] used acrylic cells to investigate visually gas evolution in an operating DMFC. They studied the effect of operating parameters and flow-bed design on gas management. It was concluded that an increase in inlet flow rate is beneficial to gas removal. Using a 5 cm^2 transparent cell, Lu and Wang [4] investigated the effects of backing pore structure and wettability on cell polarization characteristics and two-phase flow dynamics. They found that an anode backing layer of uniform pore size and high hydrophilicity is preferred for gas management in the anode. Tüber et al. [5] compared the performance of PEMFCs and DMFCs with serpentine, parallel and new fractal flow-fields. The results indicated that serpen-

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doi:10.1016/j.jpowsour.2006.07.071

Nomenclature

C	mass fraction (kg kg^{-1})
D	diffusion (m^2 s^{-1})
F	Faraday constant (C mol^{-1})
g	acceleration (m s^{-2})
H	membrane thickness (m)
h	channel height (m)
I	current density (A m^{-2})
I_0	exchange current density (A m^{-2})
I_e	ionic current density (A m^{-2})
j_L	capillary-diffusional flux of the liquid phase (kg m^{-2} s^{-1})
k	permeability of porous material (m^2)
K	distribution of the components
L	molar flow rate (mol s^{-1})
M	molecular weight (kg mol^{-1})
N	mass flux (kg m^{-2} s^{-1})
n	number of electrons
n_d	electro-osmotic drag coefficient
p	pressure (Pa)
s	stoichiometric coefficient
S	area (m^2)
T	temperature (K)
u	velocity (m s^{-1})
$U_0^{O_2}$	thermodynamic equilibrium potentials of oxygen reduction (V)
U_0^{MeOH}	thermodynamic equilibrium potentials of methanol oxidation (V)
v	water velocity (m s^{-1})
V_{cell}	cell voltage (V)
V_{anode}	volume of anode channels (m^3)
x	molar fraction in liquid phase (mol mol^{-1}); coordinate, (m)
y	molar fraction in gas phase (mol mol^{-1}); coordinate, (m)
z	coordinate (m)

Greek symbols

Γ_G	source of mass in gas phase (kg m^{-3} s^{-1})
α_A	charge-transfer coefficient of the anode
α_C	charge-transfer coefficient of the cathode
ε	porosity (m^3 m^{-3})
ε_G	gas content (m^3 m^{-3})
γ	local fractional vaporization; kinetic factor
η	overpotential (V)
φ	potential (V)
μ	viscosity (Pa s)
γ_c	advection correction factor
ρ	density (kg m^{-3})
σ	conductivity (m)
ψ	coefficient

Subscripts

i	component
in	inlet
out	outlet
L	liquid
G	gas
A	anode
C	cathode
eff	effective
mix	mixture
DL	diffusion layer
ref	reference value
t	total
s	interface; solid
m	membrane

Superscript

k	component (MeOH, CO_2, H_2O, O_2)

tine flow-fields give both the highest and the most stable performance.

Since it is very difficult to measure directly concentration and gas content profiles in anode channels, modelling is used to study a DMFC. Argyropoulos et al. [6] developed a model to predict the local pressure and chemical composition in the anode and cathode sides of a liquid-feed DMFC. Birgersson et al. [7] presented an isothermal, two-dimensional, liquid phase model for the conservation of mass, momentum and species in the anode channel and porous media of a DMFC. The data demonstrated the relative importance of mass transfer resistance in both the flow channel and the adjacent porous backing. Mugia et al. [8] derived a multi-component, steady-state, model based on phenomenological transport equations for the catalyst layer, diffusion layer and membrane. To understand the role of model parameters, they performed a parametric study of the model together with experimental validation. A comprehensive, two-dimensional model of two-phase flow with multi-component transport and electrochemical reactions was reported by Wang and Wang [9] for a liquid-feed DMFC, including electrodes, channels and PEM separator. Kulikovsky et al. [10] constructed a two-dimensional model for a gas-fed DMFC with a new type of current-collector. Schultz and Sundmacher [11] developed a one-dimensional, dynamic model of a DMFC based on Maxwell–Stefan mass transport equations and a Flory–Huggins activity model.

Optimum flow field design is important for improving flow patterns and gas evolution in anode channels. CFD simulation is widely used for PEMFC flow-field design [12–15]. Numerical modelling provides a better understanding of the main phenomena that govern fuel cell performance. Three-dimensional modelling is important to capture performance-limiting effects such as mass transfer and gas evolution. The conventional CFD-based model of DMFC requires experimental correlations for closure of multiphase model equations prior to numerical solution. Empirical correlations limit application of conventional sub-models for gas–liquid flow in a DMFC.